

# DL-Alanine, N-methyl-N-(3-chloropropoxycarbonyl)-, pentyl ester

InChI: InChI=1S/C13H24ClNO4/c1-4-5-6-9-18-12(16)11(2)15(3)13(17)19-10-7-8-14/h11H,4-10H  
InChIKey: GGBACCKOAOQSJR-UHFFFAOYSA-N

Formula: C13H24ClNO4

SMILES: CCCCCOC(=O)C(C)N(C)C(=O)OCCCCI

Mol. weight [g/mol]: 293.79

## Physical Properties

Property code	Value	Unit	Source
gf	-312.85	kJ/mol	Joback Method
hf	-754.74	kJ/mol	Joback Method
hfus	38.69	kJ/mol	Joback Method
hvap	68.88	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.806		Crippen Method
mcvol	231.130	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
tb	698.85	K	Joback Method
tc	881.34	K	Joback Method
tf	427.98	K	Joback Method
vc	0.873	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.55	J/mol×K	698.85	Joback Method
cpg	653.37	J/mol×K	729.27	Joback Method
cpg	667.41	J/mol×K	759.68	Joback Method
cpg	680.68	J/mol×K	790.10	Joback Method
cpg	693.17	J/mol×K	820.51	Joback Method
cpg	704.91	J/mol×K	850.93	Joback Method
cpg	715.91	J/mol×K	881.34	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392777&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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